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Pushing the Boundaries of Nuclear Physics with Lattice Simulations

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We review the recent highlights of nuclear lattice effective field theory, which is continuing to push the boundaries of *ab initio* nuclear many-body calculations, both in terms of nuclear structure and nuclear reactions. Significantly, this provides a deeper understanding of key nuclear processes that produce the elements necessary for life as we know it, such as carbon and oxygen. This remarkable progress has been made possible by recent dramatic increases in HPC resources, as well as advances in computational methods and algorithmic improvements.

1 Introduction

Recent advances in high-performance computing (HPC) has enabled nuclear physics to enter a new and exciting era. Calculations of nuclear structure and reactions that were once considered nearly impossible are now being readily performed. The research performed by the NLEFT (Nuclear Lattice Effective Field Theory) collaboration is at the forefront of this development. Such calculations are *ab initio* in the sense that they use nuclear forces derived from the chiral effective Lagrangian of Quantum Chromodynamics (QCD), which is the underlying theory that describes the interactions of quarks and gluons. For few-nucleon systems, the chiral effective field theory (EFT) for the forces between two, three and four nucleons have been worked out to high orders in the chiral power counting. This force consists of long-ranged exchanges of one or more pions, and shorter ranged multi-nucleon contact interactions. By combining these EFT forces with Monte Carlo methods developed by the lattice QCD community, the NLEFT collaboration has successfully studied the properties of p-shell nuclei (such as ^{12}C and ^{16}O). These nuclei have formed the calculational boundary of more traditional nuclear many-body techniques, such as Green's function Monte Carlo.

With recent advances in the methods and algorithms of NLEFT, this boundary has been pushed further by recent *ab initio* calculations of nuclei in the sd-shell. Furthermore, the NLEFT formalism has been developed and adapted to include the treatment of nuclear reactions. This ongoing line of research is now rapidly addressing key questions related to the formation of elements, including those that enable life as we know it. In the following, we briefly review the motivation and methodology behind the NLEFT formalism. We also present recent highlights of our research and conclude with an outlook on future progress.

2 Theoretical Background of NLEFT Simulations

Nuclei are self-bound systems of nucleons (protons and neutrons). As the nucleons themselves consist of quarks and gluons, and hence are not fundamental degrees of freedom, the forces between nucleons are not completely given in terms of two-body interactions, but include three-body and higher terms. Computing the properties of multi-nucleon systems presents a very difficult challenge. The complicated structure of the interaction coupled with the quantum mechanical nature of such systems leads to an exponential growth in the computational effort as a function of the number of nucleons A. For $A \leq 4$, bound state energies and scattering phase shifts have traditionally been calculated by exact (numerical) solution of the Lippmann-Schwinger or Faddeev-Yakubowsky equations. For $A \geq 5$, well established many-body techniques have been developed, such as the no-core shell model and coupled-cluster methods. These ultimately rely on the direct diagonalisation of a large matrix M in order to solve a problem of the form $Mx = b$. As the size of M increases exponentially, the memory and processing power of currently available HPC systems are quickly exhausted, which confines such methods to systems with $A \leq 12$. In order to push beyond $A = 12$, simplifications to the interaction between nucleons as well as other *ad hoc* assumptions become necessary.

In the context of QCD, systems of quarks and gluons also exhibit exponential scaling in the number of degrees of freedom, but instead of relying on direct diagonalisation in order to calculate observables, methods have been developed to stochastically *estimate* observables. The quarks and gluons are placed on a discrete space-time lattice, and Monte Carlo sampling of the propagation of the particles is performed in order to capture the most relevant contributions to a given observable. Such "lattice QCD" calculations provide a much reduced calculational complexity. Moreover, lattice QCD calculations are fully non-perturbative and provide the only known rigorous way to compute the properties of QCD in the non-perturbative (low-energy) regime. Still, it should be kept in mind that the stochastic nature of lattice QCD induces an associated uncertainty in each calculated observable, in addition to possible issues arising from numerical sign oscillations (the "sign problem") or from an unfavourable signal-to-noise ratio.

While a formalism similar to lattice QCD is used in NLEFT calculations, in the latter case the nucleons form the degrees of freedom that propagate on the space-time lattice, such that the interactions between nucleons are provided by chiral EFT. The stochastic nature of the Monte Carlo importance sampling of the nucleons' trajectories provides a softer scaling of computational complexity with A. This, in turn, is what allows NLEFT to push the boundaries of *ab initio* calculations beyond those reached by more traditional methods.

3 Nuclear Physics on a Space-Time Lattice

In NLEFT simulations, Euclidean space-time is discretised on a torus of volume $L_s^3 \times L_t$, where L_s is the side length of the (cubic) spatial dimension, and L_t denotes the extent of the Euclidean time dimension. The lattice spacing in the spatial dimensions is denoted a, analogously to a_t in the temporal dimension. The maximal momentum on the lattice is thus $p_{\max} \equiv \pi/a$, which serves as the UV regulator of the theory. Nucleons exist as pointlike particles on the lattice sites, and the interactions between nucleons (pion exchanges and

contact terms) are treated as insertions on the nucleon world lines via auxiliary-field representations. The nuclear forces have an approximate spin-isospin SU(4) symmetry (Wigner symmetry) that is of fundamental importance in suppressing numerical sign oscillations that plague any Monte Carlo simulation of strongly interacting fermions at finite density. This is in contrast to lattice QCD, where any finite baryon chemical potential renders the Monte Carlo simulation unfeasible.

We compute the properties of multi-nucleon systems by means of the transfer matrix projection Monte Carlo method. There, each nucleon is treated as a single particle propagating in a fluctuating background of pion and auxiliary fields, the latter representing the multi-nucleon contact interactions. Due to the very strong binding between four nucleons occupying the same lattice site, we find that the convergence of the chiral EFT expansion can be greatly accelerated by means of smeared LO contact interactions. We start the Euclidean time projection from a Slater determinant Ψ_A of single-nucleon standing waves for Z protons and N neutrons (with $A = Z + N$) in a periodic cube. We then use a Wigner SU(4) symmetric Hamiltonian as a computationally inexpensive filter for the first few Euclidean time steps, which also suppresses sign oscillations dramatically. Finally, we apply the full LO chiral EFT Hamiltonian and calculate the ground state energy and other properties from the correlation function

$$Z(t) \equiv \langle \Psi_A | \exp(-tH) | \Psi_A \rangle, \tag{1}$$

in the limit of large Euclidean projection time t. Higher-order contributions, such as the Coulomb repulsion between protons and other isospin-breaking effects (due to the light quark mass difference), are computed as perturbative corrections to the LO amplitude. The properties of excited states are obtained from a multi-channel projection Monte Carlo method. In our LO lattice action, the nucleon kinetic energy and momentum-dependent smearing factors of the contact interactions are treated using $\mathcal{O}(a^4)$ improvement. Moreover, all lattice operators are included up to $\mathcal{O}(Q^3)$, where Q denotes the momentum transfer between pions and nucleons. This includes operators related to the breaking of rotational symmetry on the lattice. The strengths of such operators can be tuned to eliminate unphysical effects, such as the mixing of the ${}^3D_3$ partial wave into the ${}^3S_1$-${}^3D_1$ channel.

4 Recent NLEFT Results

We shall now discuss the highlights of selected recent NLEFT calculations, which demonstrate both the strengths of the NLEFT approach as well as recent algorithmic developments. These include the sensitivity of the triple alpha process to the variation of the fundamental physical parameters, and the *ab initio* demonstration of alpha clustering in ^{12}C and ^{16}O. On the algorithmic side, we report recent results on the restoration of rotation symmetry on the lattice, as well as a new method for ameliorating sign oscillations in Monte Carlo simulations of NLEFT.

4.1 Variation of the Fundamental Physical Parameters

A significant advantage of an *ab initio* approach to nuclear physics is that we can determine the sensitivity of key nuclear processes to changes in the fundamental physical parameters, such as the light quark mass m_q (or, equivalently, the pion mass M_π) and the

electromagnetic fine-structure constant $\alpha_{\rm em}$[1]. The only additional input required for such a calculation is knowledge of the M_π-dependence of the coefficients of the contact terms in the chiral EFT interaction between nuclei. Such knowledge enables us to determine the level of "fine-tuning" that occurs in nuclear physics, and in particular address "anthropic" questions related to the formation of life in the Universe. The production rate of carbon and oxygen via the triple-alpha process and alpha capture on carbon are of particular anthropic significance, since these elements appear to be essential to life as we know it. The only known environment where the required density, temperature, and timescale for the production of such elements exists is within the cores of red giant stars. Our NLEFT simulations have revealed that the production rates of carbon and oxygen are likely to remain stable under perturbations smaller than $\simeq 2-3\%$ in m_q or $\alpha_{\rm em}$. This result is shown in Fig. 1, together with current knowledge of the M_π-dependence of the chiral EFT interaction[2].

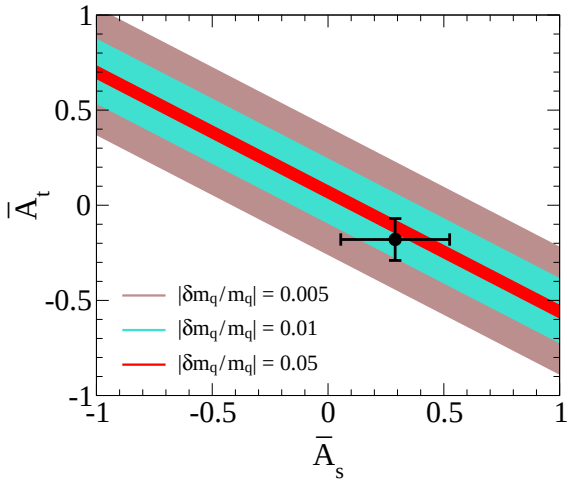

Figure 1. "Survivability bands" for carbon-oxygen based life from NLEFT simulations, due to 0.5% (broad outer band), 1% (medium band) and 5% (narrow inner band) changes in the light quark mass m_q, in terms of the slopes of the inverse NN S-wave scattering lengths a_s^{-1} and a_t^{-1}, where $\bar{A}_i \equiv \partial a_i^{-1}/\partial M_\pi$ at the physical value of the pion mass M_π. The data point with error bars represents the most recent NNLO determination of the pion mass dependence of the NN scattering lengths in chiral EFT.

4.2 Alpha Clustering in Light and Medium-Mass Nuclei

Alpha clustering within light and medium mass nuclei is an important physical phenomenon that is captured in our NLEFT simulations. Our NLEFT simulations of ^{12}C and ^{16}O, for example, provide insight into the exact configuration of alpha clustering. In the case of ^{12}C, the 0_1^+ ground state corresponds to a configuration of alpha clusters in the shape of an equilateral triangle (on the lattice an isosceles right triangle), while the 0_2^+ "Hoyle state" appears to closely resemble an obtuse triangle similar to the ozone molecule. In Fig. 2, we show the alpha clustering realised in the analogous states of ^{16}O[3]. The alpha clustering picture which emerges from NLEFT simulations is also strongly supported

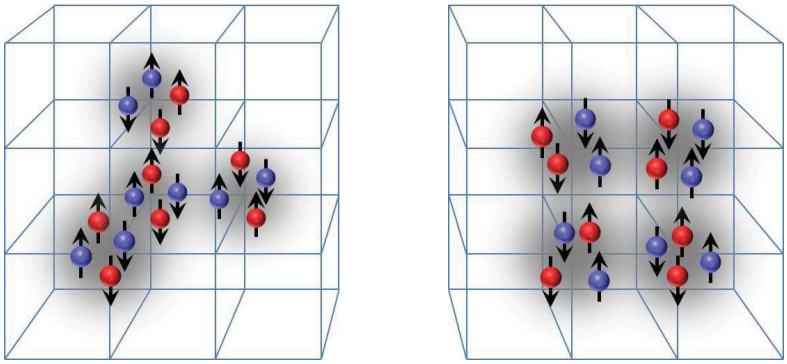

Figure 2. Illustration of alpha cluster states with tetrahedral and square configurations. The tetrahedral configuration is found to have large overlap with the 0_1^+ ground state of ^{16}O, while the square configuration corresponds closely to the excited 0_2^+ state.

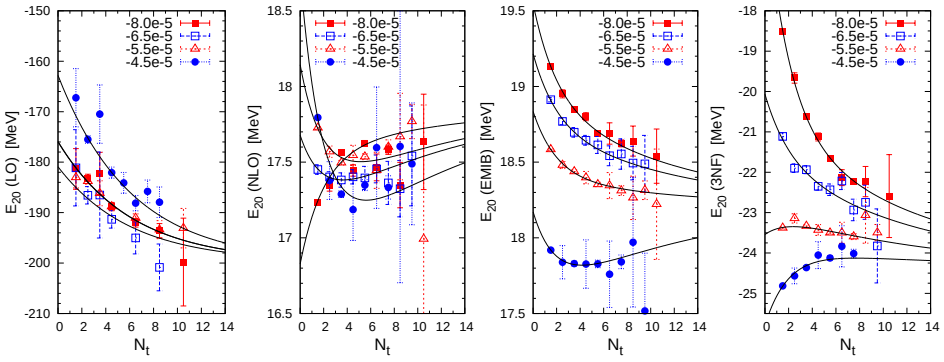

Figure 3. NLEFT simulation of the ground-state energy of ^{20}Ne to NNLO in the EFT expansion. From left to right, the contributions are the LO energy, the isospin-symmetric NLO correction, the electromagnetic and isospin-breaking (EMIB) corrections, and the three-nucleon force (3NF) correction. Contributions of NLO and higher order are treated perturbatively. The curves show a correlated fit to four different choices of the Wigner SU(4) symmetric Hamiltonian, in terms of a spectral density given by a sum of three energy delta functions. The physical results are found by extrapolation $t = a_t N_t \to \infty$.

by our results for the electromagnetic transitions between the states in question, as these are sensitive probes of the structure of the underlying wave functions. The same NLEFT simulations have also enabled the *ab initio* study of nuclei within the sd-shell, including the medium-mass nuclei ^{20}Ne, ^{24}Mg and ^{28}Si[4]. Our NLEFT simulation results for ^{20}Ne are shown in Fig. 3, including the full structure of the chiral EFT force up to NNLO in the EFT expansion. The extent of the Monte Carlo data in Euclidean time is limited by sign oscillations, which necessitates an extrapolation in order to obtain the final result for each observable.

4.3 Restoration of Rotational Symmetry on the Lattice

On the lattice, rotational invariance is broken from the full SO(3) rotational group to the cubic group. Hence, observables computed on the lattice will in general be affected by rotational symmetry breaking effects. In particular, the unambiguous identification of excited states and the computation of transition amplitudes may suffer significantly due to the relatively large lattice spacings of $a \simeq 2$ fm in present NLEFT simulations. Hence, it makes sense to carefully determine the sources of rotational symmetry breaking in actual NLEFT simulations, and search for methods that minimise their impact on physical observables. We have therefore used a simplified alpha cluster model to study the lattice matrix elements of irreducible tensor operators as a function of a[5,6].

In order to minimise the effects of rotational symmetry breaking, we have introduced the "isotropic average" which consists of a linear combination of the components of a given matrix element, such that each component is weighted according to the Clebsch-Gordan coefficient with the associated quantum numbers. This method, which is equivalent to averaging over all lattice orientations, enables the unambiguous computation of matrix elements even at large lattice spacings. In Fig. 4, we illustrate the effect of isotropic averaging on the mean square radius of ^{8}Be within the alpha cluster model.

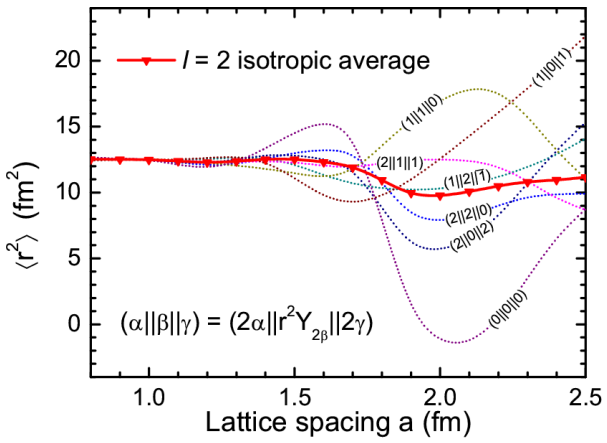

Figure 4. Mean square radii $\langle r^2 \rangle$ for the lowest 2^+ multiplet of ^{8}Be states within a simplified alpha-cluster model calculation. The reduced lattice matrix elements all merge in the limit $a \to 0$, while at finite a the matrix elements depend on the quantum number α, β and γ, which is indicative of rotational symmetry breaking. Such effects are nearly eliminated in the isotropic average, especially when $a \leq 1.7$ fm.

4.4 Combating the Sign Problem in NLEFT Simulations

While the Monte Carlo approach to NLEFT exhibits relatively mild scaling of the computational effort as a function of A, the applicability of NLEFT simulations is potentially limited by the fermionic sign oscillations inherent to the chiral EFT interaction, especially when $N \neq Z$. As already noted, the approximate Wigner SU(4) symmetry of our trial wave functions greatly alleviates the sign oscillations, which are also found to be minimised for

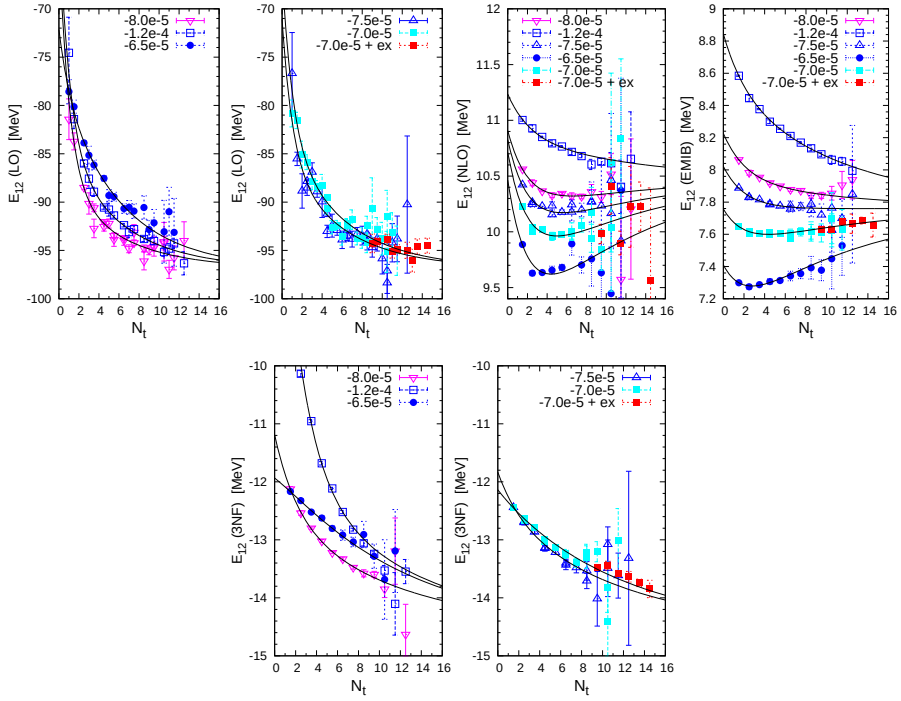

Figure 5. Updated extrapolation in Euclidean projection time for the ground state of ^{12}C, including data points (filled red squares) obtained by means of symmetry-sign extrapolation. Notation and conventions are similar to Fig. 3. The other sets of Monte Carlo data have been obtained directly at $d_h = 1$, for which simulations at $N_t = 14$ and $a_t = 1.32$ fm would be out of the question due to severe sign oscillations.

the alpha nuclei. Likewise, the momentum-dependent smearing of the LO interactions and the perturbative treatment of NLO and higher order corrections allow the sign problem to be circumvented further. Nevertheless, substantial extrapolation in Euclidean time remains necessary, which introduces additional uncertainties into the results. In order to reliably access larger nuclei as well as neutron-rich halo nuclei, we have developed a systematic approach called "Symmetry-sign extrapolation" (SSE) which allows us to perform NLEFT simulations for nuclei for which the sign problem is more severe[7].

In the SSE method, Monte Carlo simulations are performed for the Hamiltonian $H_{\rm SSE}$, given by

$$H_{\rm SSE} \equiv d_h H_{\rm phys} + (1 - d_h) H_{\rm SU(4)}, \tag{2}$$

where $H_{\rm phys}$ is the full NLEFT Hamiltonian, $H_{\rm SU(4)}$ is an SU(4) symmetric Hamiltonian which (for most cases of interest) is free of a sign problem, and $0 \leq d_h \leq 1$ is an adjustable parameter. By taking $d_h < 1$, we can always decrease the sign oscillations to a tolerable level, at the price of introducing an extrapolation $d_h \to 1$ in addition to $t \to \infty$. An additional constraint is provided by the requirement that the limit $d_h \to 1$ be independent of the choice of $H_{\rm SU(4)}$. In Fig. 5, we show how the SSE method allows us to extend the

region in Euclidean projection time accessible to Monte Carlo simulations. Clearly, SSE provides us with a valuable tool for extending the boundaries of NLEFT simulations to the regime of neutron-rich halo nuclei and to nuclei near drip lines.

5 Future of NLEFT Simulations

At this time, NLEFT has matured into a well-established *ab initio* framework at the forefront of modern theory of nuclear structure and reactions. The ongoing development of both theory and algorithms is expected to provide further insight into a number of key problems, and to further extend the applicability of NLEFT to heavier nuclei. For example, NLEFT is well placed to address the issue of possible P-wave pairing in neutron matter, which would modify the nuclear equation of state and hence the cooling rate of neutron stars. Significant progress has also been achieved in applying NLEFT to nuclear reactions using the "adiabatic projection" method to reduce a complicated many-fermion problem to a computationally simpler cluster-cluster scattering problem[8]. These investigations pave the way for *ab initio* studies of processes relevant for stellar astrophysics, such as alpha-alpha scattering, alpha-carbon scattering and radiative capture. In particular, a model-independent calculation of the "holy grail" of nuclear astrophysics, *i.e.* the $^{12}\mathrm{C}(\alpha,\gamma)^{16}\mathrm{O}$ reaction at stellar energies, appears to be within reach. In short, NLEFT appears headed toward an exciting time of progress and discovery.

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References

1. U.-G. Meißner, Sci. Bull. (2015) **60**(1):43-54 [arXiv:1409.2959 [hep-th]].
2. E. Epelbaum, H. Krebs, T. A. Lähde, D. Lee and U.-G. Meißner, Eur. Phys. J. A **49** (2013) 82 [arXiv:1303.4856 [nucl-th]].
3. E. Epelbaum, H. Krebs, T. A. Lähde, D. Lee, U.-G. Meißner and G. Rupak, Phys. Rev. Lett. **112** (2014) 10, 102501 [arXiv:1312.7703 [nucl-th]].
4. T. A. Lähde, E. Epelbaum, H. Krebs, D. Lee, U.-G. Meißner and G. Rupak, Phys. Lett. B **732** (2014) 110 [arXiv:1311.0477 [nucl-th]].
5. B. N. Lu, T. A. Lähde, D. Lee and U.-G. Meißner, Phys. Rev. D **90** (2014) 3, 034507 [arXiv:1403.8056 [nucl-th]].
6. B. N. Lu, T. A. Lähde, D. Lee and U.-G. Meißner, Phys. Rev. D **92** (2015) 1, 014506 [arXiv:1504.01685 [nucl-th]].
7. T. A. Lähde, T. Luu, D. Lee, U.-G. Meißner, E. Epelbaum, H. Krebs and G. Rupak, Eur. Phys. J. A **51** (2015) 7, 92 [arXiv:1502.06787 [nucl-th]].
8. M. Pine, D. Lee and G. Rupak, Eur. Phys. J. A **49** (2013) 151 [arXiv:1309.2616 [nucl-th]].